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The Importance of the Interaction Radius Between Cr and Self-interstitial Fe in Object Kinetic Monte Carlo Calculations of Irradiated FeCr Diluted Alloys

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We have studied electron irradiation and annealing of FeCr alloys in the dilute limit (less than 1% Cr) using Object kinetic Monte Carlo (OKMC) with input from density functional theory calculations and empirical potentials. The results are compared to experimental measurements of electric resistivity for different Cr concentrations. We analyse the dependence of Cr on the first two observed peaks: ID2 and IE and the influence of parameters such as the interaction radius between Cr and an Fe self-interstitial.

Parameters for OKMC model

Migrating species:

I up to size 4, V up to size 4
ICr 0.23 eV
I_2Cr 0.30 eV
ICr_2, I_2Cr_2 do not migrate

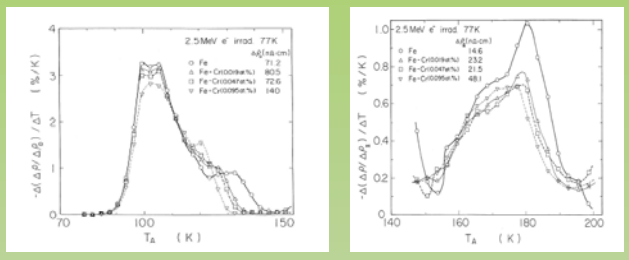
Dissociation of clusters

$ICr \rightarrow I + Cr$ 0.08 + 0.34 = 0.42 eV
$ICr_2 \rightarrow ICr + Cr$ 0.08 + 0.23 = 0.31 eV
$I + Cr_2$ 0.394 + 0.34 = 0.73 eV
$I_2Cr \rightarrow ICr + I$ 0.65 + 0.23 = 0.88 eV
$I_2 + Cr$ 0.02 + 0.43 = 0.45 eV
$I_2Cr_2 \rightarrow I_2Cr + Cr$ 0.062 + 0.30 = 0.362 eV
And others of higher energies

Simulation conditions

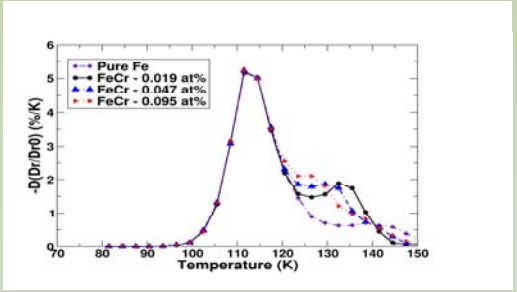
Electron irradiation at 77 K
Isochronal anneal from 77 to 200K, Heating rate 3K/3min
Pure Fe & FeCr at 0.019 at.%, 0.047 at.% & 0.095 at.%

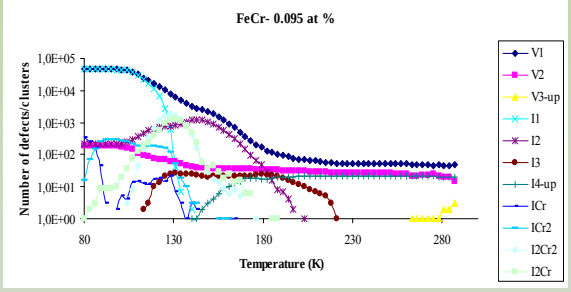
Experimental results from Abe & Kuramoto [1]



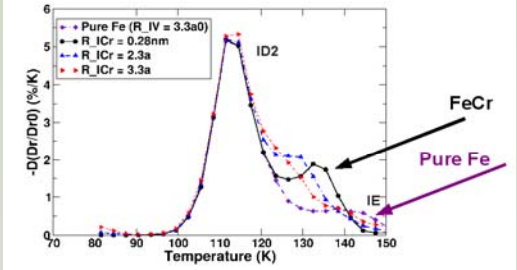
- Shift of stage IE to lower temperatures in FeCr
- Decreases in temperature and increases in amplitude with increasing Cr concentration
- Peak at 180K does not depend on solute concentration

Simulation results

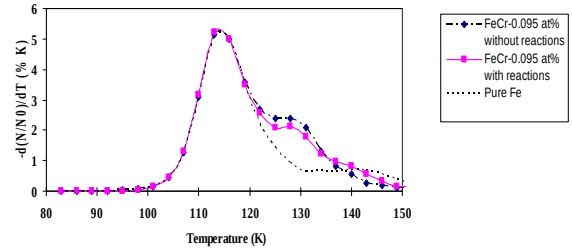




Influence of the capture radius between I an Cr on the simulation results: case of 0.019% Cr



Influence of the reactions to for ICr_2 and I_2Cr_2: case of 0.095% Cr



Conclusions: The model reproduces the shift of stage IE towards lower temperatures when Cr concentration increases. This peak is related to the formation of ICr and ICr_2 clusters. ICr migrates and recombines with V while ICr_2 dissociates into ICr and Cr. Since ICr migrates faster than an Fe interstitial the shift towards lower temperatures is reproduced. The position of the IE peak depends strongly on the ICr capture radius, with a capture radius of 0.28nm providing the best agreement with the experimental measurements. There is not a significative difference in the results when the I_2Cr and I_2Cr_2 reactions are not included. Further work is underway to study the behaviour at higher temperatures.

References.-

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